

Isopentyl alcohol
123-51-3 | DTXSID3025469

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.25e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.48e-01

Confidence level: 9.82e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isopentyl alcohol

Measured: 1.31e-11

Predicted: 1.25e-11

[Image not found](#)

1-Hexanol

Measured: 1.25e-11

Predicted: 1.24e-11

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Pentan-2-ol

Measured: 1.18e-11

Predicted: 1.20e-11

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3-Pentanol

Measured: 1.22e-11

Predicted: 1.20e-11